Symmetries and Degeneracies when T=0 Two Body Matrix Elements are Set Equal to Zero

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Abstract

The effect of setting all T=0 two body interaction matrix elements equal to a constant (or zero) in shell model calculations in the $f_{7/2}$ region are investigated. Despite the apparent severity of such a procedure, one gets fairly reasonable spectra. It is noted that using $V^{T=0} = 0$ in single j shell calculations degeneracies appear e.g. the $I = \frac{1}{2}^-$ and $\frac{13}{2}^-$ states in ^{43}Sc are at the same excitation energies as are the I=3_2^+,7_2^+,9_1^+ and 10_1^+ states in ^{44}Ti. Thus for these states the actual deviation from degeneracy are good indicators of the effects of the T=0 matrix elements. The best way of seeing the effects of the T=0 interaction in an even - even nucleus is to compare the energies of state with states of odd angular momentum with those that are even.

I. INTRODUCTION

In the early 1960's single j shell calculations in the $f_{7/2}$ region were performed by McCullen, Bayman, and Zamick (MBZ) [1,2] and Ginocchio and French[3]. In these calculations the two body matrix elements were taken from experiment. However the T=0 neutron proton spectrum in ^{42}Sc was not well determined. Calculations with correct T=0 matrix elements were later performed by Kutschera, Brown, and Ogawa[4].

In order to see how neutron-proton two body matrix elements with isospin T=0 affect the low lying spectra of nuclei, we have set them to a constant in a single j shell calculation in the $f_{7/2}$ region. We can then write $V^{T=0} = c(1/4 - t_1 \cdot t_2)$ where c is a constant. Hence $\sum_{i<j} V_{ij}^{T=0} = c/8(n(n-1)+6) - c/2T(T+1)$. This means that the spectrum of states of a given isospin e.g. T=0 in ^{44}Ti is independent of what the constant is, it might as well be zero. What the constant is will affect only the energy splittings of states with different isospin. We shall denote this matrix element input as $< T = 0 >= 0$.

Although setting all T=0 matrix elements to a constant may seem like a severe approximation, it will be seen that one gets a fairly good representation of the spectrum. When the T=0 matrix elements are reintroduced, there is some fine tuning which improves the spectrum.

While the problem of T=1 pairing is better understood and studied, there has nevertheless been a very extensive literature on the possibility of T=0 pairing, both pro and con. We here include some of the relevant references.[5-13]

In a shell model calculation the effects of both T=0 and T=1 pairing are automatically included. The problem then is to sort out as much as possible the individual effects.

In the next section we will consider calculations in which up to t nucleons are excited from the $f_{7/2}$ shell. Of course t=0 corresponds to a single j configuration.

II. RESULTS OF SINGLE J SHELL CALCULATIONS

In the following tables we show T=T_{min} calculated yrast spectra for ^{43}Ti(Table I), ^{44}Ti(Table II), and ^{46}V(Table III) where we use 4 different sets of matrix elements. Model I consists of matrix elements from ^{42}Sc. Model II consists of the FPD6 interaction [14] t=0. Model III is $< T = 0 >= 0$ for the ^{42}Sc matrix elements. Model IV is $< T = 0 >= 0$ for the FPD6 t=0. Also to gain some insight into how configuration mixing affects our results, in Table IV and V we present full fp space results for ^{43}Ti and ^{44}Ti respectively.

In the single j shell calculation for which the matrix elements were taken from the spectrum of ^{42}Sc the values of these matrix elements were 0.000 MeV, 0.6110 MeV, 1.5863 MeV, 1.4904 MeV, 2.8153 MeV, 1.5101 MeV, 3.242 MeV, and 0.6163 MeV for J=0 to 7 respectively. Note that the J=1^+ and 7^+ are nearly degenerate near 0.6 MeV and the J=3^+ and 5^+ are nearly degenerate near 1.5 MeV. Thus the act of setting T=0 matrix elements to a constant is equivilant to moving the J=1^+ and 7^+ together up to about 1.5 MeV. Or putting it another way, the act of removing the degeneracy is lower the energies of the J=1^+ and 7^+ by about the same amount. This is in contrast to most studies in which only the effects of lowering the J=1^+ state are studied.

We will point out several features to be found in the tables. We observe many levels that were considerably separated in the 'normal' interaction become degenerate when we go to $< T = 0 >= 0$. We explore this further in the next section. We find that in general with few exceptions that the odd I levels of ^{44}Ti and ^{46}V are at a lower excitation energy when we go to the $< T = 0 >= 0$ version of the interactions and that the ^{43}Ti spectra is lowered in total.

III. THE DEGENERACYS THAT OCCUR IN $< T = 0 >= 0$ AND EXPLANATIONS

As can be seen from Tables I-III some energy levels are degenerate when the T=0 matrix elements are set equal to a constant. The degenerate pairs (I_1, I_2) include

^{43}Ti $(\frac{1}{2}^-, \frac{13}{2}^-)(\frac{17}{2}^-, \frac{19}{2}^-)$

^{44}Ti $(9^+, 10^+)$

^{46}V $(12^+, 13^+)$

Let us first consider $(\frac{1}{2}^-, \frac{13}{2}^-)$ in ^{43}Ti. The basis states can be written as $[J_p, j_n]^I$ where J_p is the angular momentum of the two protons. The interaction matrix element $< [J'_p, j_n]^I V [J_p, j_n]^I >= \delta_{J'_p, J_p} E_{J_p} + 2\Sigma_J U(jjIj, J'_p J) U(jjIj, J_p J) E_J$ where E_J is the two particle matrix element $< [jj]^J V [jj]^J >$. For even J, T is equal to one while for odd J, T is equal to zero.

The wavefunctions for the Titanium isotopes are written as

$$\psi = \Sigma D^{I\alpha}(J_p, j_n)[(j^2)^{J_p}(j^n)^{J_n}]^{I\alpha} \tag{1}$$

where $D^{\pm}(J_p, j_n)$ is the probability amplitude that in a state of total angular momentum I the protons couple to J_p and the neutrons to j_n. The elements $D^I(J_p, j_n)$ form a column vector.

It is instructive to look at the energies and wavefunctions (ie column vectors) for the $I = \frac{1}{2}^-$ and $I = \frac{13}{2}^-$ states that appear in the NYO Technical reports (which included T=0 matrix elements.)

		$I = \frac{1}{2}$	$I = \frac{13}{2}$	
Energy(MeV)		5.4809	3.8477	5.8122
J_p	j_n			
4	7/2	1.000	0.9942	-0.1076
6	7/2	0.000	0.1076	0.9942

In the $f_{7/2}$ model the $I = \frac{1}{2}^-$ configuration is unique $[J_p = 4\ J_n = \frac{7}{2}]^{\frac{1}{2}-}$. There are two configurations for the $I = \frac{13}{2}^-$ state $[4\frac{7}{2}]$ and $[6\frac{7}{2}]$.

When we go to $< T = 0 >= 0$ what basically happens is that the eigenvalues and eigenfunctions become

		$I = \frac{1}{2}$	$I = \frac{13}{2}$	
		E_1	E_1	E_2
J_p	j_n			
4	7/2	1.000	1.000	0.000
6	7/2	0.000	0.000	1.000

In order for this to happen the matrix element $< [J_{p=4}, j_{n=\frac{7}{2}}]^{I=\frac{13}{2}} V [J_{p=6}, j_{n=\frac{7}{2}}]^{I=\frac{13}{2}} >$ must vanish. This vanishing is carried by the Racah coefficients $U(\frac{7}{2}\frac{7}{2}\frac{13}{2}\frac{7}{2}; 4J) U(\frac{7}{2}\frac{7}{2}\frac{13}{2}\frac{7}{2}; 6J)$ where J is the angular momentum of a neutron-proton pair.

In general J can be 4,5,6,7. However in $< T = 0 >= 0$, only even J's contribute i.e. J=4 or J=6. In either case one of the Racah coefficients will be $U(\frac{7}{2}\frac{7}{2}\frac{13}{2}\frac{7}{2}; 46)$. This Racah coefficient is zero. This guarantees a decoupling of $[4\frac{7}{2}]$ from $[6\frac{7}{2}]$ but does not in itself lead to a degeneracy of the $I = \frac{1}{2}$ and $I = \frac{13}{2}$ states. That happens because of this additional condition

$$U(\frac{7}{2}\frac{7}{2}\frac{13}{2}\frac{7}{2}; 44) = U(\frac{7}{2}\frac{7}{2}\frac{1}{2}\frac{7}{2}; 44) = \frac{1}{2} \tag{2}$$

We next consider the degeneracy of $I = 9^+$ and 10^+ in ^{44}Ti in $< T = 0 >= 0$. It is again instructive to write down the eigenfunctuions as they appear in the NYO report

		$I = 9$			$I = 10$		
Energy		8.7799	8.8590	11.5951	7.8429	9.8814	10.5110
Isospin			T=1	T=1			T=1
J_p	j_n						
4	6	-0.7071	0.5636	-0.4270	0.7037	-0.0696	0.7071
6	4	0.7071	0.5636	-0.4270	0.7037	-0.0696	-0.7071
6	6	0.0000	0.6039	0.7971	0.0984	0.9951	0.0000

Before proceeding, we remind the reader of a general rule that can clearly be seen in the wave functions above. For even total angular momentum I the wave functions of even T states of N=2 nuclei are symmetric under the interchange of neutrons and protons and the T=1 states are anti-symmetric. For odd I it is the opposite. This can be summarized by $D^{IT}(J_P, J_N) = (-1)^{I+T} D^{IT}(J_N, J_P)$.

We focus on the T=0 states. This makes the life much simpler. Instead of three states each we need only worry about one I=9 and two I=10 states. Note that for I=9 T=0 the state was the simple wavefunction $\begin{pmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$.

What clearly happens for I=10 in $< T = 0 >= 0$ is that there is a decoupling of (6,4) and (4,6) from (6,6) So that the wavefunctions of the two T=0 states become $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ and the eigenvalues of the first one becomes the same as that of the unique I=9 state.

We further note that aside from the yrast degeneracies there are other degenerices. For example, the 7_2^+ and 3_2^+ are degenerate with the I=9_1,10_1 pair in ^{44}Ti. At first this is puzzling because the dimensions are different. There are seven basis states for I=3 and six for I=7, whereas for I=9 and 10 there are only three basis states. However, of the seven I =3 states, five have isospin <u>one</u>, and only two have isospin T=0. Of the six I=7 states, four have isospin one and only two have isospin zero. Since we are focusing on T=0 we only show only these wavefunctions in Table VI. When the T=0 two particle matrix elements are set equal to zero the wave functions simplify as shown in the table.

We now begin to see a connections between $I = 3_2^+, 7_2^+, 9_1^+, 10_1^+$. For the 9_1^+ and 10_1^+ the only non-zero components of the wave function in the $< T = 0 >= 0$ are D(4,6) and D(6,4) both having magnitude $\frac{1}{\sqrt{2}}$. The 3_1^+ state has nonzero components D(2,4) and D(4,2). There is no connection with the 9_1^+ and 10_1^+ states. However for the 3_2^+ state the only non-vanishing matrix elements are D(4,6) and D(6,4) each with magnitude $\frac{1}{\sqrt{2}}$. This is the same as what occurs for the 9_1^+ and 10_1^+ states.

A similar story is written by I=7. The non vanishing components for the 7_1^+ state in the $< T = 0 >= 0$ case are D(2,6) and D(6,2) however for the 7_2^+ state they are D(4,6) and D(6,4) each with magnitude $\frac{1}{\sqrt{2}}$.

Thus a common theme emerges for $I = 3_2^+, 7_2^+, 9_1^+, 10_1^+$ (all T=0) in that for the $<$

$T = 0 >= 0$ case the only non-vanishing components of the wave functions are D(4,6) and D(6,4). Visually, the column vectors look the same. And it is precisely these states that are degenerate.

Although in Table VI we have only shown T=0 wave functions there are several T=1 states interspaced amongst the T=0 states. For example, in the Technical Report NYO-9891 [2] for I=3 the lowest state calculated to be at 6.2357 MeV has T=1. The calculated energy for this state is about 300 keV lower than the lowest T=0 state shown in Table VI. Other T=1 states are calculated to be at 9.2334, 10.0321 and 10.9022 MeV. For I=7 the lowest T=1 state is calculated to be at 6.7094 MeV, just above the other the lowest T=0 state shown in Table VI. The other T=1 states for I=7 are calculated to be at 9.0744, 9.5141 and 12.1535 MeV. The closeness of T=0 and T=1 states was previously discussed by Goode and Zamick [15].

IV. FULL F-P CALCULATION FOR ^{43}TI AND ^{44}TI

We have performed full fp calculations for ^{43}Ti and ^{44}Ti with the FPD6 interaction.

Let us first compare the full calculation for ^{43}Ti (Table IV , first column of energy levels) with the single j shell calculation of Table I (Model II). One sees systematic deviations. The states with I less than $\frac{7}{2}$ come down in energy while those with I greater than $\frac{7}{2}$ go up in energy when the full fp calculation is performed. The $\frac{1}{2}^-$, $\frac{3}{2}^-$ and $\frac{5}{2}^-$ states come down respectively 2.304,1.807, and 1.328 MeV. What is very probably happening is that one is going in the direction of forming a K=1/2- rotational band.

We next make a comparison of full fp results using FPD6 and FPD6 $< T = 0 >= 0$. These results for ^{43}Ti are shown in Table IV.

For I greater than $\frac{7}{2}$ every other spin gets its energy raised by a substantial amount when the T=0 interactions are turned back on i.e. for I=$\frac{9}{2}$,$\frac{13}{2}$ and $\frac{17}{2}$ the increases in excitation energies are respectively 0.663,0.647, and 1.104 MeV respectively. However for $\frac{11}{2}$ and $\frac{15}{2}$ there are decreased -0.111 and -0.117 MeV. Thus the effect of the T=0 interaction is to introduce a staggering.

Perhaps one striking fact is that when the T=0 matrix elements are set to zero the $\frac{15}{2}^-$ and $\frac{13}{2}^-$ are nearly degenerate with respective excitation energies of 3.065 and 3.070 MeV–only 0.005 MeV splitting.In the more realistic case when the T=0 matrix elements are put back in the splitting increases to 0.770 MeV. But one still has to look hard and in some detail to find the effects of the T=0 matrix elements. We next consider the full f-p calculation for ^{44}Ti.

In Table V we show the effects of configuration mixing on ^{44}Ti. As configuration mixing is turned on in $< T = 0 >= 0$, the formerly degenerate states I=9,10 remain close. Further, the I=3,5 and I=7,8 states which were relatively close in the $< T = 0 >= 0$ t=0 calculation remain close. Comparing with the FPD6 with $< T = 0 >$ included we see that I=3,5 started close and drifted apart as configuration mixing was turned on while I=7,8 are never close in the presence of nonzero T=0 matrix elements.

Comparing the $< T = 0 >= 0$ FPD6 with the regular FPD6 for ^{44}Ti in Table V we see that the odd I states are at a much higher energy when T=0 matrix elements are included. The excitation energy difference is much larger in a t=4 calculation than in a t=0 calculation. For example the J=9 state in a full fp is 1.96 MeV higher when T=0 matrix elements are not set equal to zero whereas in a t=0 calculation it is only 0.201 MeV higher. So configuration mixing is important for getting the odd spin - even spin energy difference.

Work on the effect of L=0, T=1 and L=1, T=0 pairing in the f-p shell has already been performed by Poves and Martinez-Pinedo.[16] They start with a realistic interaction, KB3, and study the effects of removing the T=1 pairing the the T=0 S=1 pairing. They focused on binding energies and on the even spin states of ^{48}Cr. Relative to their work, whose conclusions we certainly agree with, we have made a more severe approximation of setting all T=0 matrix elements equal to zero. The payoff for us is that certain degeneracies appear between states, the deviation of which in the physical spectrum can largely be attributed to T=0 two body matrix elements. Also, we focussed on odd I excited states. The deviation in the physical spectrum of the energies of odd I states from even I is also a good indication of the effects of T=0 matrix elements.

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TABLES

TABLE I. Spectra of ^{43}Ti

Model I		Model II		Model III		Model IV	
I	E(MeV)	I	E(MeV)	I	E(MeV)	I	E(MeV)
7/2	0.0000	7/2	0.000	7/2	0.000	7/2	0.000
9/2	1.680	9/2	1.247	9/2	1.640	9/2	1.444
11/2	2.335	11/2	1.439	3/2	1.831	3/2	1.558
3/2	2.888	19/2	1.652	11/2	2.061	11/2	1.709
5/2	3.449	15/2	1.867	5/2	2.832	5/2	2.187
13/2	3.500	13/2	2.099	1/2	3.279	13/2	2.435
15/2	3.511	3/2	2.678	13/2	3.279	1/2	2.435
19/2	3.644	17/2	2.696	15/2	3.425	15/2	2.541
17/2	4.298	5/2	3.633	17/2	3.919	17/2	2.902
1/2	4.316	1/2	4.147	19/2	3.919	19/2	2.902

TABLE II. Spectra of ^{44}Ti

Model I		Model II		Model III		Model IV	
I	E(MeV)	I	E(MeV)	I	E(MeV)	I	E(MeV)
0	0.000	0	0.000	0	0.000	0	0.000
2	1.163	2	0.958	2	1.303	2	1.203
4	2.790	4	1.973	4	2.741	4	2.133
6	4.062	6	2.870	6	3.500	6	2.602
3	5.786	8	3.785	3	4.716	3	3.771
5	5.871	12	3.963	5	4.998	5	3.971
7	6.043	10	4.132	7	5.356	7	4.241
8	6.084	7	4.537	8	5.656	8	4.418
10	7.384	5	4.562	9	7.200	9	5.357
12	7.702	3	4.675	10	7.200	10	5.357
9	7.984	9	5.161	12	7.840	12	5.825

TABLE III. Spectra of ^{46}V

Model I		Model II		Model III		Model IV	
I	E(MeV)	I	E(MeV)	I	E(MeV)	I	E(MeV)
5	0.000	7	0.000	3	0.000	5	0.000
1	0.169	5	0.114	1	0.007	3	0.042
3	0.256	6	0.119	5	0.048	1	0.198
6	0.547	3	0.875	6	0.514	7	0.247
7	0.783	9	0.960	7	0.610	6	0.471
4	1.516	4	1.175	4	1.017	4	0.765
2	2.185	1	1.227	2	1.157	2	0.842
9	2.456	8	1.239	9	2.419	9	1.665
8	2.669	11	1.898	8	2.534	8	1.737
11	4.310	2	2.197	10	4.192	10	2.810
10	5.001	10	2.721	11	4.212	11	2.836
13	6.745	13	3.061	12	6.715	13	4.776
12	7.608	15	3.688	13	6.715	12	4.776
15	8.704	12	3.835	15	8.726	15	6.053

TABLE IV. ^{43}Ti full fp calculation

FPD6		FPD6 $< T = 0 >= 0$	
I	E(MeV)	I	E(MeV)
7/2	0.000	7/2	0.000
3/2	0.871	3/2	1.668
1/2	1.805	9/2	1.970
11/2	1.889	11/2	2.000
5/2	2.305	5/2	2.638
9/2	2.633	1/2	2.940
15/2	2.948	15/2	3.065
19/2	3.401	13/2	3.070
13/2	3.718	17/2	3.325
17/2	4.429	19/2	3.417

TABLE V. ^{44}Ti full fp calculation

FPD6		FPD6 $< T = 0 >= 0$	
I	E(MeV)	I	E(MeV)
0	0.000	0	0.000
2	1.317	2	1.515
4	2.536	4	2.587
6	3.843	6	3.223
3	6.241	3	4.717
8	6.383	5	4.932
5	7.579	8	5.292
10	7.790	7	5.391
7	7.921	10	6.476
12	8.574	9	6.574
9	9.030	1	7.070
1	9.681	12	7.192
11	11.028	11	9.914

TABLE VI. Comparison of wave functions of MBZ[a] with those for which $< T = 0 >= 0$ matrix elements are set equal to zero.

I=3		MBZ	$< T = 0 >= 0$	MBZ	$< T = 0 >= 0$
Energy(MeV)		6.533		10.493	
J_P	J_N				
2	2	0.0000	0	0.0000	0
2	4	0.6968	$\frac{1}{\sqrt{2}}$	-0.1202	0
4	2	-0.6968	$\frac{-1}{\sqrt{2}}$	0.1202	0
4	4	0.0000	0	0.0000	0
4	6	0.1202	0	0.6968	$\frac{1}{\sqrt{2}}$
6	4	-0.1202	0	-0.6968	$\frac{-1}{\sqrt{2}}$
6	6	0.0000	0	0.0000	0
I=7		MBZ	$< T = 0 >= 0$	MBZ	$< T = 0 >= 0$
Energy(MeV)		6.5723		9.6570	
J_P	J_N				
2	6	0.6965	$\frac{1}{\sqrt{2}}$	0.1220	0
4	4	0.0000	0	0.0000	0
4	6	0.1220	0	-0.6965	$\frac{-1}{\sqrt{2}}$
6	2	-0.6965	$\frac{-1}{\sqrt{2}}$	-0.1220	0
6	4	-0.1220	0	0.6965	$\frac{1}{\sqrt{2}}$
6	6	0.0000	0	0.0000	0
I=9		MBZ	$< T = 0 >= 0$	MBZ	$< T = 0 >= 0$
Energy(MeV)		8.7799			
J_P	J_N				
4	6	-0.7071	$\frac{-1}{\sqrt{2}}$		
6	4	0.7071	$\frac{1}{\sqrt{2}}$		
6	6	0.0000	0		
I=10		MBZ	$< T = 0 >= 0$	MBZ	$< T = 0 >= 0$
Energy(MeV)		7.8429		9.8814	
J_P	J_N				
4	6	0.7037	$\frac{1}{\sqrt{2}}$	-0.0696	0
6	4	0.7037	$\frac{1}{\sqrt{2}}$	-0.0696	0
6	6	0.0084	0	0.9951	1

a) From Technical Report NYO 9801 [2]

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